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M.R.H. Rudge, et al

Douglas Advanced Research Laboratories
Huntington Beach, California

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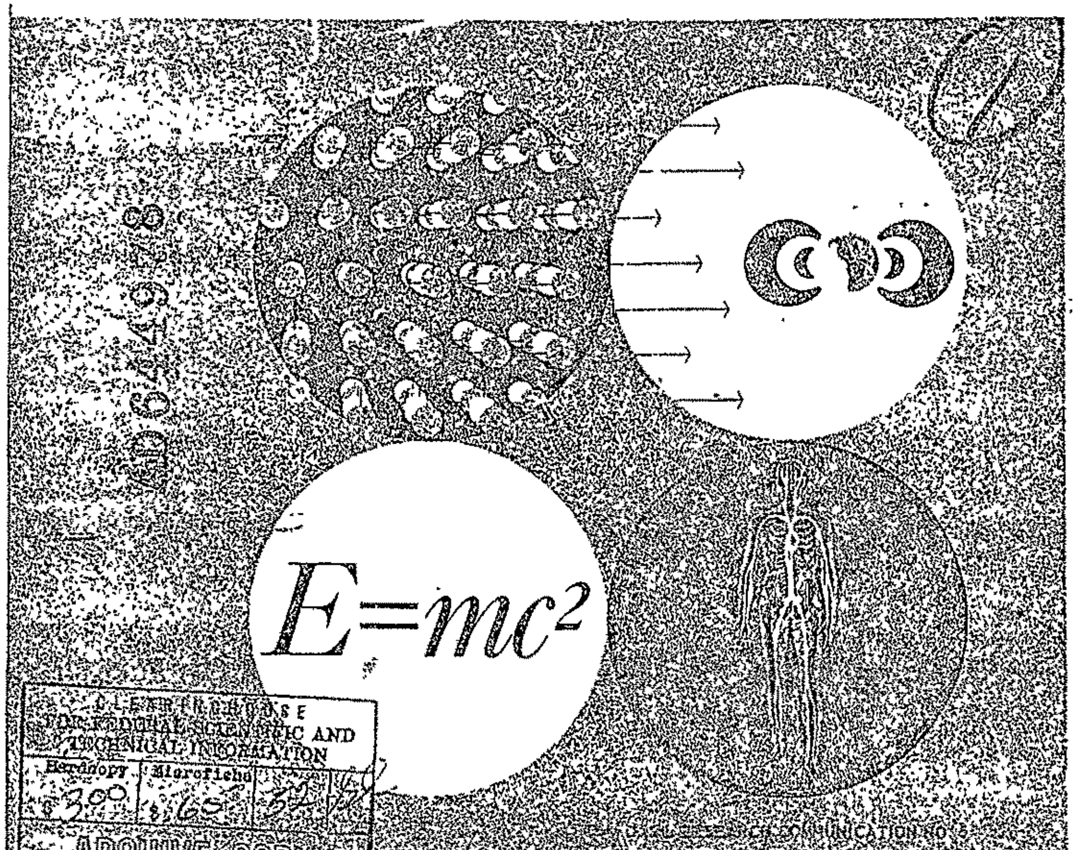

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M.R.H. RUDGE

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FEBRUARY 1966

DOUGLAS

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THE IONIZATION OF HYDROGEN AND OF HYDROGENIC POSITIVE IONS BY ELECTRON IMPACT

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ABSTRACT

Calculations of the ionization cross sections of hydrogen and of hydrogenic positive ions are described in which the initial state is either the ground or the excited 2s state. The first procedures used are the Born (ii) and Born-exchange approximations. These results are compared with other theoretical calculations and with experimental data. It is seen that for the case of ionization of hydrogen from its ground state, none of the theoretical results is in good agreement with the experimental data. A certain defect of the theory is then corrected by adopting a third procedure for this case, in which an angle-dependent Coulomb potential is used in the description of the final state of the e-H ionization problem. It is then found that, despite the sounder theoretical footing of this latter calculation, no improved agreement with experimental data is obtained except in the near threshold region.

Convenient formulae are presented which represent the best data for the ionization cross sections and the associated reaction rates for the case of an initial Maxwellian distribution of velocities.

CONTENTS

ILLUSTRATIONS

TABLES

1. INTRODUCTION

Considerable interest attaches to an accurate knowledge of ionization cross sections both in astrophysical work and in studies of laboratory plasmas. In some cases experimental data are available, in particular for the ionization cross section of atomic hydrogen from its ground state and for He^+ from its ground state. Certain species of interest, however, for example the highly ionized iron ions such as Fe^{+14}, are not readily susceptible to experimental investigation, and this is true also of ionization from excited states. Our main interest lies with the calculation of ionization cross sections in these cases. In this paper however, we confine our attention to ionization in the hydrogen isoelectronic sequence from the ground state and from the excited 2s state. The species considered are hydrogen, He^+ and a fictitious hydrogenic ion with nuclear charge $Z = 128$.

Three approximations have been considered. The first of these, the Born (ii) approximation, has been previously used by Rudge and Seaton (1965) in the calculation of the ionization cross section of atomic hydrogen from its ground state. The calculations presented here have extended the use of this approximation to the other cases, and since we repeat the ground state hydrogen work also, we therefore have a ready check on the accuracy of our program. This program, written to encompass calculations for an arbitrary atom or ion with the theory expressed in terms of partial wave expansions, gives a typical agreement with the results of Rudge and Seaton (1965) of about 0.1%, the latter results having been obtained without recourse to such expansions. To achieve this accuracy, however, has involved a very much greater amount of computation than that undertaken by Burgess and Rudge (1963) in their partial wave calculations. In our second procedure, therefore, the Born-exchange approximation, we have repeated the work of Burgess and Rudge (1963) on ground state He^+, obtaining more accurate results, and again extended the application of this method to the other ions. We first of all compare the results of these two approximations, Born (ii) and Born-exchange, with the Born (i), Born-Oppenheimer and 'close-coupling' results presented by Burke and Taylor (1965). An indication of the relative merits of the various theoretical procedures may be seen for the cases of the ionization of H or He^+ from their ground states where experimental data are available for comparison.

For the case of He^+ the Born-exchange calculations give excellent agreement with the experimental data. For the case of H, however, in neither the Born-exchange approximation, in which simple functions are adopted in both the initial and final states, nor in the approximation of Burke and Taylor (1965), in which an improved initial state wave function is used, does good agreement obtain. It is of interest therefore to consider the effect of improving the description of the final state. In all calculations of ionization cross sections hitherto, this has been incorrectly treated as regards the Coulomb potentials, and might be expected to have a significant effect on the cross section calculation. The theory showing what asymptotic description of the final state should be employed in ionizing collisions has been given by Peterkop (1962) and by Rudge and Seaton (1965). We have therefore considered a third approximation which is in accord with this theory and investigated what effect this has on the calculation of the ionization cross section for ground state hydrogen.

The results of the calculations are shown in tabular and graphical form, and we present also sets of coefficients which provide fits to the cross sections and to the associated reaction rates.

2. THEORY

The theory of ionizing collisions has been considered by Peterkop (1961, 1962) and by Rudge and Seaton (1965). Here we summarize the arguments leading to the cross section expressions we have used.

Consider the process in which an atom or ion, intially in a state specified by $\psi(n,\underline{r})$, is ionized by an electron whose initial momentum is $\underline{k}_n$ and whose final momentum is $\underline{k}$, the momentum of the ejected electron being $\underline{\chi}$. Then, using atomic units, denoting the Hamiltonian of the system by H, the total positive energy by E and the nuclear charge by Z, an exact integral expression for the direct scattering amplitude is given by

$$f(\underline{\chi},\underline{k}) = -(2\pi)^{-5/2} \exp i\left(\Delta(\underline{\chi},\underline{k})\right)\int \Psi^*(\underline{r}_1,\underline{r}_2)(H-E)\Phi(\underline{r}_1,\underline{r}_2)\,d\underline{r}_1 d\underline{r}_2 \qquad (1)$$

where

$$\Delta(\underline{\chi},\underline{k}) = \frac{2z}{\chi}\ln\frac{\chi}{X} + \frac{2z'}{k}\ln\frac{k}{X} \qquad (2)$$

with

$$X = \sqrt{2E}$$

and

$$\frac{z}{\chi} + \frac{z'}{k} = \frac{Z}{\chi} + \frac{Z}{k} - \frac{1}{|\underline{\chi}-\underline{k}|} \qquad (3)$$

In (1), $\Psi(\underline{r}_1,\underline{r}_2)$ is the total wave function of the system and is subject to the usual boundary conditions, while $\Phi(\underline{r}_1,\underline{r}_2)$ is a function having the asymptotic form

$$\Phi(\underline{r}_1,\underline{r}_2) \underset{\substack{r_1\to\infty \\ r_2\to\infty}}{\sim} \phi(z,-\underline{\chi},\underline{r}_1)\,\phi(z',-\underline{k},\underline{r}_2) \tag{4}$$

where

$$\phi(z,\underline{k},\underline{r}) = \exp\left(\frac{\pi\eta}{2}\right)\Gamma(1-i\eta)\,e^{i\underline{k}\cdot\underline{r}}\,{}_1F_1\left(i\eta,1,i(kr-\underline{k}\cdot\underline{r})\right) \tag{5}$$

with

$$\eta = \frac{z}{k}$$

Given the exact direct scattering amplitude $f(\underline{\chi},\underline{k})$, the exact exchange amplitude is given by

$$g(\underline{\chi},\underline{k}) = f(\underline{k},\underline{\chi}) \tag{6}$$

Alternatively, one may interchange $\underline{r}_1$ and $\underline{r}_2$ in one of the wave functions appearing in the integral expression (1) and again obtain the exchange scattering amplitude. On averaging over spins, the total ionization cross section is then given by

$$Q(E) = \frac{1}{k_n}\int_0^{E/2} k\chi\, d\left(\frac{\chi^2}{2}\right)\int \sigma(\underline{\chi},\underline{k})\,d\hat{\chi}\,d\hat{k} \tag{7}$$

where

$$\sigma(\underline{\chi},\underline{k}) = \left[4\pi(2\ell_1+1)\right]^{-1}\sum_{m_1}\int d\underline{\hat{k}}_n\left[|f(\underline{\chi},\underline{k})|^2 + |g(\underline{\chi},\underline{k})|^2 - \mathrm{Re}\left(f(\underline{\chi},\underline{k})\,g^*(\underline{\chi},\underline{k})\right)\right] \tag{8}$$

with ℓ_1, m_1 the angular quantum numbers of the state $\psi(n,\underline{r})$.

Expression (1) may be properly used only if the requirement (3) is satisfied, in which case the relative phase of the resulting direct and exchange scattering amplitudes is uniquely specified. If on the other hand equation (3) is not satisfied, then there exists an essential arbitrariness in the relative phase. We do not therefore agree with the assertion of Burke and Taylor (1965), that simply by formulating the problem in terms of singlet and triplet amplitudes the phase factor problem disappears. In their calculations, as in the first of those described in this paper, the condition (3) is not met, and accordingly there are two distinct approximations, one for the magnitude of the scattering amplitudes and another for their relative phase. In the Born-exchange approximation we have adopted the same phase choice as Burgess and Rudge (1963), this having been found to give excellent agreement with the experimental data for ionization of ground state He^{+}. Explicitly the direct scattering amplitude has been written as

$$f(\underline{\chi},\underline{k}) = -(2\pi)^{-5/2}\int \psi(n,\underline{r}_1)\phi(z-1,\underline{k}_n,\underline{r}_2)\left(\frac{1}{r_{12}} - \frac{I}{r_2}\right)\phi(z,-\underline{\chi},\underline{r}_1)$$
$$\phi(z-1,-\underline{k},\underline{r}_2)d\underline{r}_1 d\underline{r}_2 \tag{9}$$

which, using standard partial wave expansions [e.g., Burgess and Rudge (1963)], may be written

$$f(\underline{\chi},\underline{k}) = -2^{7/2}\pi^{1/2}(k_n k\chi)^{-1/2} \sum_{\substack{\ell_1' m_1' \\ \ell_2' m_2' \\ \ell_2 m_2 \\ L\, M \\ \lambda}} \Big\{ \exp i\mu(\ell_2,\ell_1',\ell_2') Y^*_{\ell_2 m_2}(\hat{\underline{k}}_n) Y_{\ell_2' m_2'}(\hat{\underline{k}}) Y_{\ell_1' m_1'}(\hat{\underline{\chi}})$$
$$\cdot C^{\ell_1' \ell_2' L}_{m_1' m_2' M}\, C^{\ell_1 \ell_2 L}_{m_1 m_2 M}\, f_\lambda(\ell_1,\ell_2,\ell_1',\ell_2',L) T_\lambda(\ell_1,\ell_2,\ell_1',\ell_2';\chi,k) \Big\} \tag{10}$$

where

$$\mu(\ell_2,\ell_1',\ell_2') = \frac{\pi}{2}(\ell_2-\ell_1'-\ell_2') + \arg\Gamma\left(\ell_2+1-i\frac{z-1}{k_n}\right) + \arg\Gamma\left(\ell_2'+1-i\frac{z-1}{k}\right)$$
$$+ \arg\Gamma\left(\ell_1'+1-i\frac{z}{\lambda}\right) \tag{11}$$

$$f_\lambda(\ell_1,\ell_2,\ell_1',\ell_2';L) = \langle \ell_1\ell_2 L | P_\lambda(\hat{\underline{r}}_1\cdot\hat{\underline{r}}_2) | \ell_1'\ell_2' L\rangle \tag{12}$$

[Percival and Seaton (1958)]

and

$$T_\lambda(\ell_1,\ell_2,\ell_1',\ell_2';\chi,k) = \int_0^\infty F_{\ell_2}(z-1,k_n,r_2)F_{\ell_2'}(z-1,k,r_2)y_\lambda(\chi,\ell_1',r_2)dr_2 \tag{13}$$

with

$$y_\lambda(\chi,\ell_1',r_2) = r_2^{-(\lambda+1)}\int_0^{r_2} r^\lambda P_{n,\ell_1}(r)F_{\ell_1'}(z,\chi,r)dr$$
$$+ r_2^\lambda \int_{r_2}^\infty r^{-(\lambda+1)} P_{n,\ell_1}(r)F_{\ell_1'}(z,\chi,r)dr \tag{14}$$

In (14), $P_{n,\ell_1}(r)$ is the radial function for the bound state, while the regular Coulomb functions $F_\ell(z,k,r)$ satisfy

$$\left[\frac{d^2}{dr^2} + k^2 + \frac{2z}{r} - \frac{\ell(\ell+1)}{r^2}\right]F_\ell(z,k,r) = 0 \tag{15}$$

The exchange scattering amplitude is given in the Born-exchange approximation by

$$g(\underline{\chi},\underline{k}) = \exp i\delta(\underline{\chi},\underline{k}) f(\underline{\nu},\underline{\chi}) \tag{16}$$

where we choose $\delta(\underline{\chi},k)$ such that in expressions for the cross section there is no dependence on the phase factors $\mu(\ell_2,\ell_2',\ell_1')$. We then obtain the result that

$$\int\sigma(\underline{\chi},\underline{k})\,d\hat{\underline{\chi}}\,d\hat{\underline{k}} = \frac{2^5}{k_n k\chi}\sum_{\substack{L,\ell_2,\\ \ell_1',\ell_2'}}{}' (2L+1)\left\{\left[\sum_\lambda f_\lambda(\ell_1,\ell_2,\ell_1',\ell_2',L)T_\lambda(\ell_1,\ell_2,\ell_1',\ell_2';\chi,k)\right]^2\right.$$

$$+\left[\sum_\lambda f_\lambda(\ell_1,\ell_2,\ell_2',\ell_1';L)T_\lambda(\ell_1,\ell_2,\ell_2',\ell_1';k,\chi)\right]\cdot \tag{17}$$

$$\cdot\left[\sum_\lambda f_\lambda(\ell_1,\ell_2,\ell_2',\ell_1';L)T_\lambda(\ell_1,\ell_2,\ell_2',\ell_1',k,\chi)\right.$$

$$\left.\left. - (-1)^{\ell_1+\ell_2-L}\sum_\lambda f_\lambda(\ell_1,\ell_2,\ell_1',\ell_2',L)T_\lambda(\ell_1,\ell_2,\ell_1',\ell_2',\chi,k)\right]\right\}$$

Equations (7) and (17) give the ionization cross section in the Born-exchange approximation, while neglect of all the exchange terms leads to the Born (ii) approximation. Omitting just the interference term in (17) leads to the Born (i) approximation.

These approximations, though useful, are, as has been noted, defective in that the final state is not correctly described, i.e., equation (3) is not satisfied. We therefore consider a new approximation in which we retain the approximation that $\Psi(\underline{r}_1,\underline{r}_1) = \psi(n,\underline{r}_1)\,\phi\,(z-1,\underline{k}_n,\underline{r}_2)$ but define $\Phi(\underline{r}_1,\underline{r}_2)$ by the equation,

$$\Phi(\underline{r}_1,\underline{r}_2) = \phi(z,-\underline{\chi},\underline{r}_1)\phi(z',-\underline{k},\underline{r}_2) \tag{18}$$

with

$$z = 1$$

and

$$z' \equiv z'(\underline{\chi},\underline{k}) = 1 - \frac{k}{|\underline{\chi}-\underline{k}|} \tag{19}$$

Thus the scattering amplitude may be written in this approximation as

$$f(\underline{\chi},\underline{k}) = -(2\pi)^{-5/2}\exp i\Delta(\underline{\chi},\underline{k})\int\Psi(\underline{r}_1,\underline{r}_2)\,\frac{1}{r_{12}}\,\Phi(\underline{r}_1,\underline{r}_2)\,d\underline{r}_1\,d\underline{r}_2 \tag{20}$$

Using spherical harmonic expressions for the wave functions we then find, after some algebra, that

$$\sigma_d(\underline{\chi},\underline{k}) = 2^5\,\frac{(k_n k\chi)^{-1}}{(4\pi)^2}\sum_{\substack{\ell_2 L q\\ \ell_1' L_1' \ell_2' L_2'\\ \lambda\ \lambda'}}\left\{\cos\left[\alpha(\underline{\chi},\underline{k})\right](2L+1)(2q+1)\right.$$

$$f_\lambda(\ell_1,\ell_2,\ell_1',\ell_2';L)f_{\lambda'}(\ell_1,\ell_2,L_1',L_2';L)f_q(\ell_1',\ell_2',L_1',L_2';L) \tag{21}$$

$$\left.\cdot T_\lambda(\ell_1,\ell_2,\ell_1',\ell_2',\underline{\chi},\underline{k})T_{\lambda'}(\ell_1,\ell_2,L_1',L_2';\underline{\chi},\underline{k})P_q(\hat{\underline{\chi}}\cdot\hat{\underline{k}})\right\}$$

In (21), $P_q(x)$ is a Legendre polynomial, and the radial integrals T_λ are defined by equations (13) and (14), with the difference, however, that $z-1$ is replaced by z' defined by equation (19). $\alpha(\underline{\chi},\underline{k})$ is a phase factor given by

$$\alpha(\underline{\chi},\underline{k}) = \gamma(\ell_1',\ell_2',\underline{\chi},\underline{k}) - \gamma(L_1',L_2',\underline{\chi},\underline{k}) \tag{22}$$

where

$$\gamma(\ell_1',\ell_2',\underline{\chi},\underline{k}) = \frac{\pi}{2}(\ell_1'+\ell_2') + \arg\Gamma\left(\ell_1'+1-\frac{i}{\chi}\right) + \arg\Gamma\left(\ell_2'+1-\frac{iz'(\underline{\chi},\underline{k})}{k}\right) \tag{23}$$

Since the phase factors are defined in this treatment of the problem, we have the result that

$$\sigma_e(\underline{\chi},\underline{k}) = \sigma_d(\underline{k},\underline{\chi}) \tag{24}$$

while

$$\begin{aligned}\sigma_{int}(\underline{\chi},\underline{k}) = 2^5\left[\frac{(k_n k\chi)}{(4\pi)^2}\right]^{-1} \sum_{\substack{\ell_2 L q\\ \ell_1' L_1'\\ \ell_2' L_2'\\ \lambda\ \lambda'}} \Big[(-1)^{L_1'+L_2'-L}\cos\left[\delta(\underline{\chi},\underline{k})\right](2L+1)(2q+1)\\ \cdot f_\lambda(\ell_1,\ell_2,\ell_1',\ell_2';L)\,f_{\lambda'}(\ell_1,\ell_2,L_1',L_2';L)\,f_q(\ell_1',\ell_2',L_2',L_1',L)\\ \cdot T_\lambda(\ell_1,\ell_2,\ell_1',\ell_2';\underline{\chi},\underline{k})\,T_{\lambda'}(\ell_1,\ell_2,L_1',L_2';\underline{k},\underline{\chi})\,P_q(\hat{\underline{\chi}}\cdot\hat{\underline{k}})\Big]\end{aligned} \tag{25}$$

where

$$\delta(\underline{\chi},\underline{k}) = \Delta(\underline{\chi},\underline{k}) - \Delta(\underline{k},\underline{\chi}) + \gamma(\ell_1',\ell_2',\underline{\chi},\underline{k}) - \gamma(L_1',L_2',\underline{k},\underline{\chi}) \tag{26}$$

Substitution of equations (21), (24) and (25) into (7) gives the final expression for the cross section, which we write

$$Q(E) = \int_0^{E/2} d\left(\frac{\chi^2}{2}\right)\int_{-1}^{1} I(\underline{\chi},\underline{k})\,d(\hat{\underline{\chi}}\cdot\hat{\underline{k}}) \tag{27}$$

where

$$\begin{aligned} I(\underline{\chi},\underline{k}) &= \frac{8\pi^2\chi k}{k_n}\,\sigma(\underline{\chi},\underline{k})\\ &= I_d + I_e + I_{in}\end{aligned} \tag{28}$$

the three terms of (28) corresponding to those of (8). The calculation of the cross section in this approximation thus involves one more numerical integration than do the Born (ii) and Born-exchange approximations.

On neglecting the effects of exchange, we retain only the term I_d to give a non-exchange cross section, which we label Q_d.

3. NUMERICAL PROCEDURES

The Coulomb functions were generated by a power series near the origin to the first inflection point and thereafter by numerical integration with a step length in r of $\frac{2^{-8}n}{Z}$, where n is the principal quantum number. The routine was written generally for the case in which the Coulomb potential was modified by a short-range potential, in which case the normalization cannot be fixed a priori by means of the power series. The method of Strömgren described by Seaton and Peach (1962) was therefore adopted.

The functions $y_\lambda(\chi,\ell,r)$ were generated by numerical integration using Simpson's rule with a step length in r of $\frac{2^{-5}n}{Z}$. The final quadrature in the calculation of $T_\lambda(\ell_1,\ell_2,\ell_1',\ell_2';\underline{\chi},\underline{k})$ was again calculated using Simpson's rule, but, due to the long tail of the integral, an acceleration procedure was devised which has previously been described (Rudge and Schwartz 1965). Simpson's rule was found for these integrals to be more accurate than higher-order Newton-Cotes formulae.

The Racah and Clebsch-Gordon coefficients needed in the calculation were generated in the program. All summations were carried through to convergence except for that on L, which was terminated when sufficient values had been obtained to make an accurate extrapolation possible. It should perhaps be mentioned that in using a Gauss scheme to evaluate the angular integration in (27), care had to be exercised in deciding the convergence of the q summation of equation (25) due to the explicit occurrence of the Legendre polynomial in that sum. Due to the large amount of computation involved in evaluating the expression (27), the number of Gauss points in the angular integration was restricted to four. This should not, however, involve any substantial error.

4. RESULTS

We express all our results as reduced cross sections defined by

$$Q_R(E/I) = \frac{1}{n}\left(\frac{I}{I_H}\right)^2 Q(E/I)$$

where

I = the ionization potential

I_H = the ionization potential of hydrogen

$Q(E/I)$ = the ionization cross section in units of πa_o^2

n = the effective number of electrons (one in this case)

In table I we show results for the reduced cross sections for ionization from the 1s state of the various hydrogenic ions in the Born (ii) and Born-exchange approximations. In the case of hydrogen there have been a number of experimental measurements [Fite and Brackmann (1958), Boyd and Boksenberg (1960) Rothe et al. (1962) and McGowan and Fineman (1965)]. We are indebted to the latter authors for making their data available to us prior to publication. The 'experimental' data with which we compare our results were obtained by taking what we believe to be a reasonable interpolation amongst all these measurements. For He^+ the data are those of Dolder, Harrison and Thonemann (1961). Table II shows the results for ionization from the 2s state, and in tables III and IV are shown the contributions to the various cross sections arising from individual values of the total angular momentum. We found it convenient to fit our results to an expression of the form

$$Q_R(E/I) = \frac{\ln(E/I)}{E/I}\left[A_o + \frac{A_1}{E/I} + \frac{A_2}{(E/I)^2}\right] \qquad (29)$$

The parameters A_0, A_1 and A_2 are displayed in table V. For H 1s and He^+ 1s the coefficients were obtained from the experimental data, while in other cases the Born-exchange results were fitted. Expression (29) has the virtue of having the correct functional form both at threshold and at very high energies. We have also fitted the reaction rate defined by

$$K = \int_0^\infty vQ(E)\phi(v)dv$$

where $\phi(v)$ is the Maxwell distribution. Defining $\alpha = I/kT$ with k = Boltzmann's constant and T the absolute temperature, we write

$$10^8 K = n\left(\frac{I_H}{I}\right)^{3/2} e^{-\alpha} \sum_{m=o}^{5} K_m\alpha^m \ \mathrm{cm}^3\ \mathrm{sec}^{-1}$$

The coefficients K_m are displayed in table VII and give a fit accurate to about 5% in the range α = 0.2 to 10.0 .

In figure (i) we display the various theoretical results for the ionization of the 1s state of H

compared with the experimental results. The data are not new in this case; the Born (i) and Born (ii) curves have been taken from the work of Rudge and Seaton (1965), and our present Born results agree with those data to better than 0.1%. The B.e. results are those presently calculated, and the close-coupling and B.O. results are those of Burke and Taylor.

For the case of He^+ 1s, it is clear from table I that the Born-exchange results are in excellent accord with the experimental data. A comparison of this result with the close-coupling results of Burke and Taylor (1965) has been previously given (Rudge and Schwartz 1965).

In figure (ii) we compare the various theoretical results for ionization of H from the 2s state. We see that both the Born-exchange and close-coupling results predict that the effect of exchange is to increase the cross section in this case in contrast to the 1s ionization results. In the low-energy region there is a substantial difference between the theoretical results, however. Figure (iii) shows the results for He^+ 2s. In figure (iv) we show the behavior of the ionization cross section from the 2s state in the Born (ii) and Born-exchange approximations. The behavior of the two approximations as regards scaling is seen to differ in contrast to the case of ionization from the 1s state, where the results of both approximations increase with increasing Z. Figure (iv), showing the scaling in the 2s case, may be compared with figure (v), which shows the scaling for the 1s case, where the hydrogen curve and the He^+ curves are experimental (the latter coinciding with Born-exchange results) and the upper curve is for $Z = 128$.

In table VI we show results of calculations of the ionization cross section of hydrogen from its ground state using the angle-dependent potential. In this table, H_1 is the Gauss weight for the energy integration and H_2 is that for the angular integration. $z'(\underline{X},\underline{k})$ and $z'(\underline{k},\underline{X})$ are the charges defined by equation (19), the former being used in calculations of the direct scattering amplitude and the latter in calculations of the exchange scattering amplitude. We show the contribution to the cross section arising from each ejected energy and each angle between the scattered and ejected electrons. In the angular integration, a four-point Gauss quadrature was used at all energies, and to avoid repetition we display the abscissae $\hat{\underline{X}}\cdot\hat{\underline{k}}$ and the weights H_2 for only the first entry in the table, the corresponding entries being identical for the other cases.

Table I. $Q_R(E/I)$ for Ionization from the 1s state

E/I	Z=1, Born(ii)	Z=2, Born(ii)	Z=128, Born(ii)	Z=1 B.e.	Z=2 B.e.	Z=128 B.e.	Z=1 Experimental	Z=2 Experimental
1.125	-----	0.215	-----	-----	0.213	-----	0.12	0 19
1.25	-----	0.392	0.466	-----	0 366	0 477	0.21	0.33
1.50	0.465	0.666*	0.744	0.476	0.580*	0.720	0.36	0.53*
2.25	0.876	1.002	1.074	0.804	0.834	0.975	0.60	0 81
3.0	0.997	1.072	1.119	0.889	0.896	1.002	0.69	0.89
4.0	0.996	1.035	1.064	0.883	0.881	0.952	0.72	0.87
5.0	0.939	0.962	-----	0.836	0.832	-----	0 71	0.83

*Values for E/I = 1.51525

Table II. $Q_R(E/I)$ for Ionization from the 2s state

E/I	Z=1,Born(ii)	Z=2,Born(ii)	Z=128,Born(ii)	Z=1 B.e.	Z=2 B.e.	Z=128 B.e.
1.25	------	0.415	0.488	----	0.572	0 528
1.50	0.510	0.668	0.758	0.749	0.819	0.766
2.25	0 826	0.957	1.031	1.120	0.994	0.949
3.0	0.886	0.979	1.035	1.113	0.956	0.926
4.0	-----	0.916	0.953	-----	0.865	0.846
5.0	0.795	-----	-----	0.887	-----	------
6 0	-----	0.758	----	-----	0.704	------

Table III. Total Angular Momentum Contributions to $Q_R(E/I)$ for Ionization from the 1s state

E/I	L	H(Bii)	He^+(Bii)*	Z=128(Bii)	H(B.e.)	He^+(B.e.)*	Z=128(B.e.)
1.50	0	6.059,-2	7.415,-2	5.880,-2	4.929,-2	6.629,-2	5.143,-2
	1	1.605,-1	1.451,-1	1.026,-1	1.939,-1	1.481,-1	9.668,-2
	2	1.312,-1	2.090,-1	2.221,-1	1.318,-1	1.740,-1	2.100,-1
	3	6.811,-2	1.339,-1	1.856,-1	6.166,-2	1.073,-1	1.851,-1
	4	2.861,-2	6.382,-2	1.022,-1	2.486,-2	5.125,-2	1.037,-1
	5	1.062,-2	2.587,-2	4.556,-2	9.195,-3	2.126,-2	4.602,-2
	6	3.636,-3	9.463,-3	1.778,-2	3.194,-3	8.022,-3	1.781,-2
	7	1.180,-3	3.233,-3	6.345,-3	1.058,-3	2.829,-3	6.310,-3
	8	3.694,-4	1.055,-3	2.128,-3	3.385,-4	9.503,-4	2.108,-3
2.25	0	7.150,-2	7.366,-2	6.346,-2	5.765,-2	6.144,-2	5.157,-2
	1	1.799,-1	1.495,-1	1.155,-1	1.873,-1	1.342,-1	9.891,-2
	2	2.142,-1	2.353,-1	2.280,-1	1.990,-1	1.880,-1	1.998,-1
	3	1.701,-1	2.122,-1	2.388,-1	1.489,-1	1.686,-1	2.160,-1
	4	1.095,-1	1.460,-1	1.796,-1	9.432,-2	1.191,-1	1.682,-1
	5	6.282,-2	8.711,-2	1.131,-1	5.454,-2	7.361,-2	1.083,-1
	6	3.372,-2	4.794,-2	6.447,-2	2.981,-2	4.192,-2	6.253,-2
	7	1.740,-2	2.513,-2	3.462,-2	1.572,-2	2.266,-2	3.386,-2
	8	8.769,-3	1.280,-2	1.794,-2	8.092,-3	1.185,-2	1.764,-2
	9	4.368,-3	6.421,-3	9.099,-3	4.107,-3	6.065,-3	8.991,-3
	10	2.167,-3	3.197,-3	4.567,-3	2.070,-3	3.069,-3	4.527,-3

Table III. Total Angular Momentum Contributions to $Q_p(E/I)$
for Ionization from the 1s state (Cont.)

E/I	L	H(Bii)	He^{+}(Bii)*	Z=128(Bii)	H(B.e.)	He^{+}(B.e.)*	Z=128(B.e.)
3.0	0	5.980,-2	5.911,-2	5.289,-2	4.811,-2	4.781,-2	4.195,-2
	1	1.495,-1	1.248,-1	1.007,-1	1.435,-1	1.055,-1	8.294,-2
	2	1.991,-1	1.994,-1	1.883,-1	1.788,-1	1.582,-1	1.596,-1
	3	1.875,-1	2.066,-1	2.155,-1	1.627,-1	1.655,-1	1.887,-1
	4	1.440,-1	1.674,-1	1.867,-1	1.245,-1	1.382,-1	1.695,-1
	5	9.840,-2	1.181,-1	1.370,-1	8.603,-2	1.010,-1	1.282,-1
	6	6.285,-2	7.691,-2	9.148,-2	5.595,-2	6.792,-2	8.746,-2
	7	3.861,-2	4.782,-2	5.781,-2	3.507,-2	4.346,-2	5.608,-2
	8	2.322,-2	2.898,-2	3.541,-2	2.150,-2	2.697,-2	3.469,-2
	9	1.383,-2	1.734,-2	2.133,-2	1.303,-2	1.645,-2	2.105,-2
	10	8.217,-3	1.033,-2	1.277,-2	7.859,-3	9.946,-3	1.265,-2
4.0	0	4.458,-2	4.324,-2	3.976,-2	3.594,-2	3.433,-2	3.192,-2
	1	1.125,-1	9.539,-2	7.975,-2	1.018,-1	7.785,-2	6.440,-2
	2	1.584,-1	1.523,-1	1.427,-1	1.389,-1	1.210,-1	1.187,-1
	3	1.669,-1	1.723,-1	1.725,-1	1.442,-1	1.394,-1	1.483,-1
	4	1.455,-1	1.569,-1	1.651,-1	1.263,-1	1.310,-1	1.472,-1
	5	1.130,-1	1.250,-1	1.359,-1	9.944,-2	1.078,-1	1.251,-1
	6	8.169,-2	9.195,-2	1.019,-1	7.319,-2	8.171,-2	9.619,-2
	7	5.667,-2	6.446,-2	7.234,-2	5.172,-2	5.879,-2	6.955,-2
	8	3.842,-2	4.397,-2	4.976,-2	3.568,-2	4.100,-2	4.847,-2
	9	2.577,-2	2.960,-2	3.367,-2	2.431,-2	2.810,-2	3.309,-2
	10	1.723,-2	1.984,-2	2.263,-2	1.649,-2	1.911,-2	2.239,-2

Table III. Total Angular Momentum Contributions to $Q_p(E/I)$
for Ionization from the 1s state (Cont.)

E/I	L	H(Bii)	He^{+}(Bii)*	Z=128(Bii)	H(B.e.)	He^{+}(B.e.)*	Z=128(B.e.)
5.0	0	3.372,-2	3.248,-2	-------	2.733,-2	2.578,-2	-------
	1	8.622,-2	7.421,-2	-------	7.581,-2	5.981,-2	-------
	2	1.244,-1	1.180,-1	-------	1.078,-1	9.427,-2	-------
	3	1.391,-1	1.395,-1	-------	1.200,-1	1.139,-1	-------
	4	1.307,-1	1.359,-1	-------	1.139,-1	1.144,-1	-------
	5	1.097,-1	1.168,-1	-------	9.706,-2	1.013,-1	-------
	6	8.565,-2	9.256,-2	-------	7.710,-2	8.256,-2	-------
	7	6.396,-2	6.979,-2	-------	5.857,-2	6.376,-2	-------
	8	4.655,-2	5.110,-2	-------	4.332,-2	4.765,-2	-------
	9	3.344,-2	3.684,-2	-------	3.157,-2	3.494,-2	-------
	10	2.392,-2	2.640,-2	-------	2.287,-2	2.538,-2	-------
	11	1.713,-2	1.892,-2	-------	1.655,-2	1.839,-2	-------
	12	1.233,-2	1.362,-2	-------	1.202,-2	1.335,-2	-------

*Values for E/I = 1.51525.

Table IV. Total Angular Momentum Contributions to Q_R(E/I) for Ionization from the 2s state

E/I	L	Z=1(Bii)	Z=2(Bii)	Z=128(Bii)	Z=1(B.e.)	Z=2(B.e.)	Z=128(B.e.)
1.50	0	3.964,-2	2 196,-2	1.315,-2	3.270,-2	1.883,-2	1.131,-2
	1	4.709,-2	8.622,-2	6.614,-2	5.073,-2	8.992,-2	7.190,-2
	2	9.609,-2	9.999,-2	1.179,-1	1.607,-1	9.524,-2	1.119,-1
	3	1.171,-1	1.210,-1	9.969,-2	2 019,-1	2.308,-1	1.100,-1
	4	9.373,-2	1.211,-1	1.468,-1	1.500,-1	1.615,-1	1 395,-1
	5	5.947, 2	9.144,-2	1.209,-1	8.480,-2	1.054,-1	1.164,-1
	6	3.162,-2	6.075,-2	8 159,-2	4.026,-2	6.075,-2	8.515,-2
	7	1.468,-2	3.481,-2	5.252,-2	1.699,-2	3.100,-2	5 626,-2
	8	6.146,-3	1.741,-2	3.053,-2	6.601,-3	1.455,-2	3 291,-2
2.25	0	4.311,-2	2.812,-2	1.7105,-2	3.517,-2	2.260,-2	1.369,-2
	1	8 122,-2	9.376,-2	7 676,-2	8.004,-2	8.553,-2	7 340,-2
	2	9.895,-2	1.215,-1	1.264,-1	1.469,-1	1.094,-1	1.117,-1
	3	1.372,-1	1.296,-1	1.195,-1	2.250,-1	1.839,-1	1.188,-1
	4	1.432,-1	1.541,-1	1.564,-1	2.228,-1	1.900,-1	1 392,-1
	5	1.170,-1	1.411,-1	1.614,-1	1.672,-1	1.484,-1	1.395,-1
	6	8.278,-2	1 067,-1	1.313,-1	1.073, 1	1.005,-1	1.185,-1
	7	5.317,-2	7.275,-2	9.290,-2	6.282,-2	6.343,-2	8.788,-2
	8	3.182,-2	4.608,-2	6.103,-2	3.473,-2	3.835,-2	5.936,-2
	9	1.800,-2	2 748,-2	3 792,-2	1 847,-2	2.240,-2	3.741,-2
	10	9.747,-3	1 559,-2	2.244, 2	9 575,-3	1.270,-2	2.230,-2

Table IV. Total Angular Momentum Contributions to Q_R(E/I) for Ionization from the 2s state (Cont.)

E/I	L	Z=1(Bii)	Z=2(Bii)	Z=128(Bii)	Z=1(B e.)	Z=2(B.e.)	Z=128(B.e.)
3.0	0	3.495,-2	2.574,-2	1.685,-2	2.854,-2	2.040,-2	1.326,-2
	1	7.508,-2	7.781,-2	6.632,-2	7.045,-2	6.729,-2	6.005,-2
	2	8.960,-2	1.054,-1	1.047,-1	1.149,-1	9.352,-2	9.084,-2
	3	1.151,-1	1.117,-1	1.061,-1	1.740,-1	1.335,-1	1.007,-1
	4	1.346,-1	1.340,-1	1.310,-1	1.971,-1	1.555,-1	1.150,-1
	5	1.275,-1	1.400,-1	1.460,-1	1.737,-1	1.445,-1	1.237,-1
	6	1.026,-1	1.205,-1	1.362,-1	1.296,-1	1.137,-1	1.173,-1
	7	7.436,-2	9.118,-2	1.084,-1	8.735,-2	8.084,-2	9.692,-2
	8	5.027,-2	6.362,-2	7.797,-2	5.537,-2	5.431,-2	7.212,-2
	9	3.237,-2	4.204,-2	5.271,-2	3.379,-2	3.524,-2	4.992,-2
	10	2.009,-2	2.670,-2	3 415,-2	2.013,-2	2.231,-2	3.287,-2
4.0	0	------	2.058,-2	1.475,-2	------	1.634,-2	1.160,-2
	1	------	5.780,-2	5 088,-2	------	4 861,-2	4.466,-2
	2	------	8.066,-2	7.803,-2	------	7.106,-2	6.764,-2
	3	------	8.756,-2	8.406,-2	------	9.301,-2	7.744,-2
	4	------	1.033,-1	1.002,-1	------	1.125,-1	8.809,-2
	5	------	1.164,-1	1.152,-1	------	1.183,-1	9.778,-2
	6	------	1.132,-1	1.188,-1	------	1.077,-1	1.008,-1
	7	------	9.649,-2	1.067,-1	------	8.750,-2	9.264,-2
	8	------	7.477,-2	8.566,-2	------	6.573,-2	7.661,-2
	9	------	5.427,-2	6.368,-2	------	4.692,-2	5.845,-2
	10	------	3.769,-2	4.497,-2	------	3.241,-2	4.213,-2
	11	------	2.540,-2	3 068,-2	------	2.190,-2	2.920,-2
	12	------	1.677,-2	2.045,-2	------	1.459,-2	1 971,-2

Table V. Parameters giving a fit to the cross sections*

Atom	Initial State	A0	A_1	A_2
H	1s	2.785	-3.226	1.536
H	2s	1.910	5.487	-6.289
He^+	1s	2.962	-1.759	0.422
He^+	2s	2.137	1.489	-0.206
Z=128	1s	2.799	-0.218	0.047
Z=128	2s	2.168	1.147	-0.212

Table VI. Contributions to $Q_R(E/I)$ for ionization of ground state hydrogen, using angle-dependent potentials

E/I	x	H_1	$\hat{\chi}\cdot\hat{k}$	H_2	$z'(\underline{\chi},\underline{k})$	$z'(\underline{k},\underline{\chi})$	I_d	I_d+I_e	I
1.05	0.111803	0.025	-0.861136	0.347855	0.344553	0.621577	1.276	2.561	1.707
			-0.339981	0.652145	0.238814	0.560529	1.576	2.995	2.456
			0.339981	0.652145	-0.031006	0.404748	0.337	2.600	2.506
			0.861136	0.347855	-0.717567	8.36209,-3	≈(6,-9)	3.72,-1	3.72,-1
					$\int I(\underline{\chi},\underline{k})d(\hat{\chi}\cdot\hat{k})$	=	1.69	4.67	3.96
			Q_d=0.042			Q_d+Q_e=0.12		Q=0.10	
			Q_{Bri}=0.026			Q_{Be}=0.034		Q_{exp}=0.05	

Table VI. Contributions to $Q_R(E/I)$ for ionization of ground state hydrogen, using angle-dependent potentials (Cont.)

E/I	χ	H_1	$z'(\underline{\chi},\underline{k})$	$z'(\underline{k},\underline{\chi})$	I_d	I_d+I_e	I
1.25	0.162529	0.0625	0.235310	0.737158	1.278	2.150	1.884
			0.139931	0.704374	1.316	2.263	1.559
			-0.063332	0.634507	0.824	2.227	2.040
			-0.378609	0.526139	0.101	2.257	2.452
			$\int I(\underline{\chi},\underline{k})d(\hat{\underline{\chi}}\cdot\hat{\underline{k}})$	=	1.87	4.46	3.86
	0.313982	0.0625	0.426535	0.537272	0.996	1.875	1.407
			0.325761	0.455958	1.215	2.287	1.883
			0.047586	0.231499	1.006	2.434	2.558
			-0.955955	-0.578256	4.54,-5	4.44,-4	4.89,-4
			$\int I(\underline{\chi},\underline{k})d(\hat{\underline{\chi}}\cdot\hat{\underline{k}})$	=	1.79	3.73	3.39
			$Q_d=0.23$	$Q_d+Q_e=0.51$		$Q=0.45$	$Q_{exp}=0.21$

Table VI. Contributions to $Q_R(E/I)$ for ionization of ground state hydrogen, using angle-dependent potentials (Cont.)

E/I	χ	H_1	$z'(\underline{\chi},\underline{k})$	$z'(\underline{k},\underline{\chi})$	I_d	I_d+I_e	I
1.50	0.229850	0.125	0.235310	0.737158	1.131	1.635	2.230
			0.139931	0.704374	1.200	1.793	2.370
			-0.063332	0.634507	1.057	1.903	1.797
			-0.378609	0.526139	0.368	1.596	1.193
			$\int I(\underline{\chi},\underline{k})d(\hat{\underline{\chi}}\cdot\hat{\underline{k}})$	=	1.99	3.53	3.91
	0.444037	0.125	0.426535	0.537272	0.721	1.298	0.865
			0.325761	0.455958	0.913	1.661	1.152
			0.047586	0.231499	0.943	1.951	1.590
			-0.955955	-0.578256	3.3,-3	1.2,-2	1.2,-2
			$\int I(\underline{\chi},\underline{k})d(\hat{\underline{\chi}}\cdot\hat{\underline{k}})$	=	1.46	2.81	2.10
			$Q_d=0.43$	$Q_d+Q_e=0.79$		$Q=0.75$	$Q_{exp}=0.36$

Table VI. Contributions to $Q_R(E/I)$ for ionization of ground state hydrogen, using angle-dependent potentials (Cont)

E/I	χ	H_1	$z'(\underline{\chi},\underline{k})$	$z'(\underline{k},\underline{\chi})$	I_d	I_d+I_e	I
2.25	0.265403	0.173611	0.178167	0.799170	0.931	1.076	1.349
			0.096815	0.779270	1.019	1.207	1.561
			-0.057887	0.741486	1.194	1.437	1.838
			0.251127	0.694264	1.092	1.397	1.521
			$\int I(\underline{\chi},\underline{k})d(\hat{\chi}\cdot\hat{k})$	=	2.15	2.59	3.21
	0.559017	0.277778	0.344553	0.621577	0.414	0.572	0.432
			0.238814	0.560529	0.594	0.842	0.647
			-0.031006	0.404748	0.789	1.149	1.041
			-0.717567	0.008362	0.266	0.527	0.626
			$\int I(\underline{\chi},\underline{k})d(\hat{\chi}\cdot\hat{k})$	=	1.14	1.68	1.47
	0.744689	0.173611	0.452447	0.511042	0.244	0.442	0.271
			0.355123	0.424132	0.403	0.736	0.431
			0.083390	0.181478	0.566	1.048	0.614
			-0.963206	-0.753119	5.1,-2	0.101	6.2,-2
			$\int I(\underline{\chi},\underline{k})d(\hat{\chi}\cdot\hat{k})$	=	0.73	1.35	0.80
			Q_d=0.72	Q_d+Q_e=1.15	Q=1.10	Q_{exp}=0.60	

Table VII. Parameters giving a fit to the reaction rate $0.2 \le \alpha \le 10.0$

Atom	Initial State	K_0	K_1	K_2	K_3	K_4	K_5
H	1s	3.621	-2.063	8.036,-1	-1.681,-1	1.700,-2	-6.455,-4
H	2s	3.457	1.621	-1.638	4.840,-1	-5.836,-2	2.450,-3
He^+	1s	4.052	-1.320	2.641,-1	-1.816,-2	7.438,-4	9.448,-5
He^+	2s	3.273	1.085	-9.794,-1	2.814,-1	-3.360,-2	1.405,-3
Z=128	1s	4.013	-2.186,-1	-3.474,-1	1.338,-1	-1.769,-2	7.767,-4
Z=128	2s	3.275	8.003,-1	-8.262,-1	2.439,-1	-2.943,-2	1.238,-3

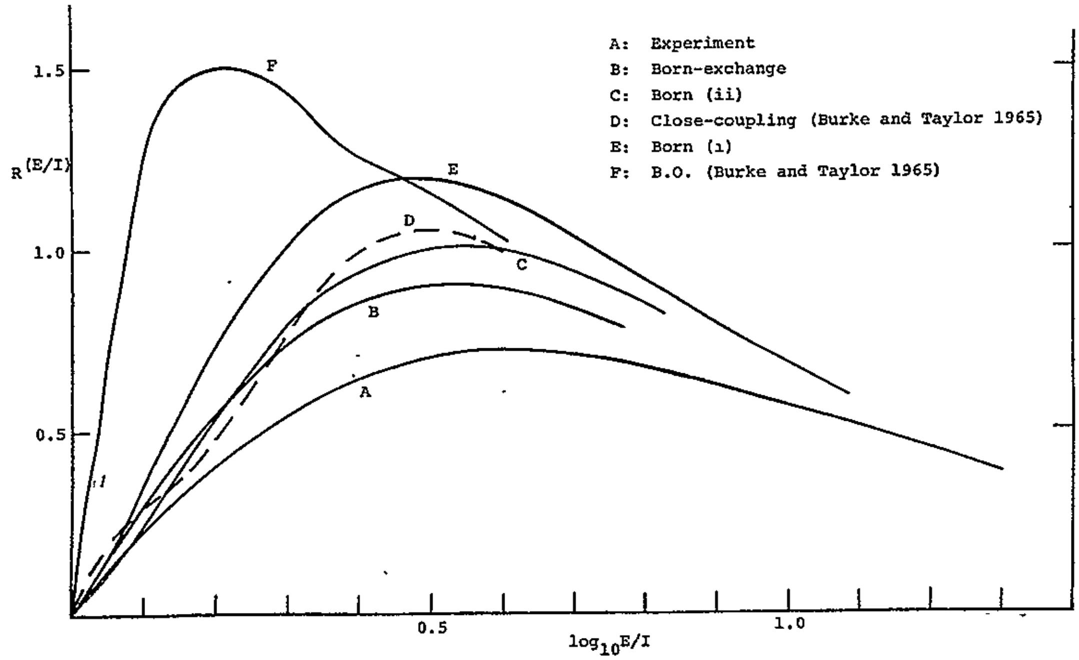

Figure (i). The ionization cross section for H (1s)

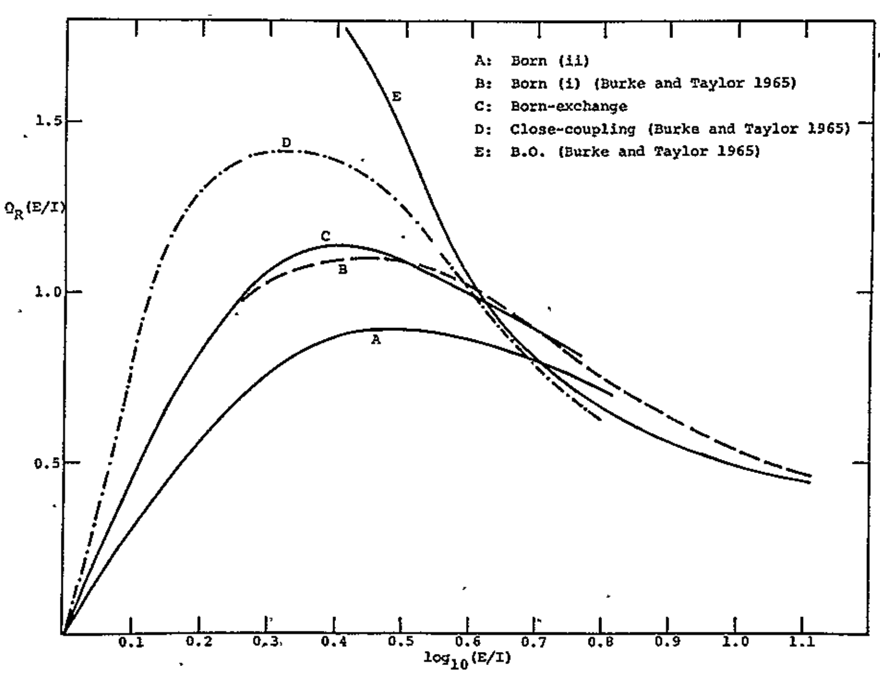

Figure (ii). The reduced ionization cross section for H 2s

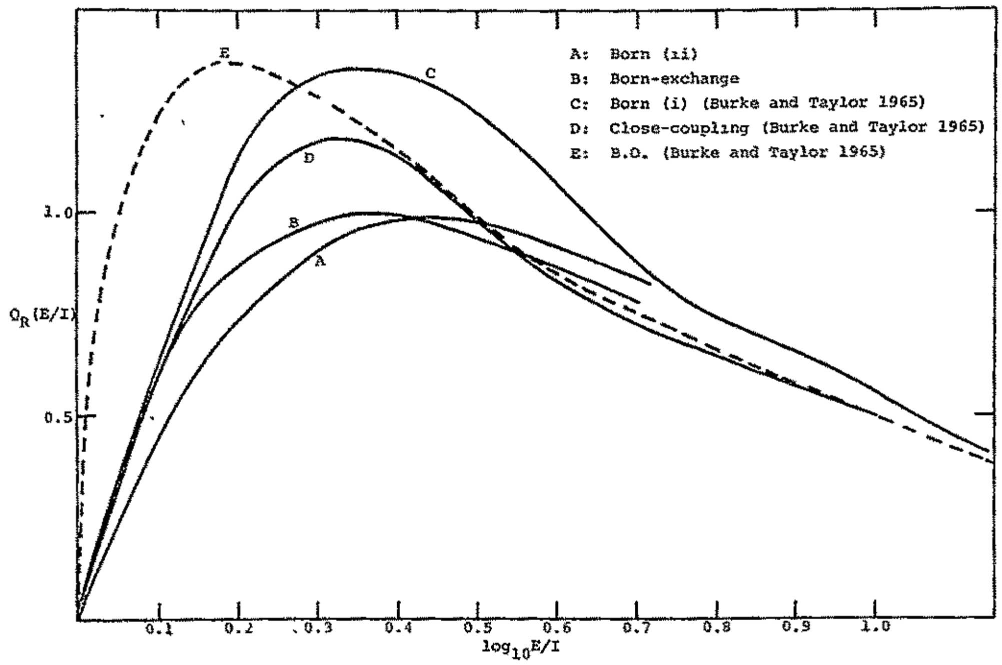

Figure (iii). The reduced ionization cross section for $He^{+}2s$

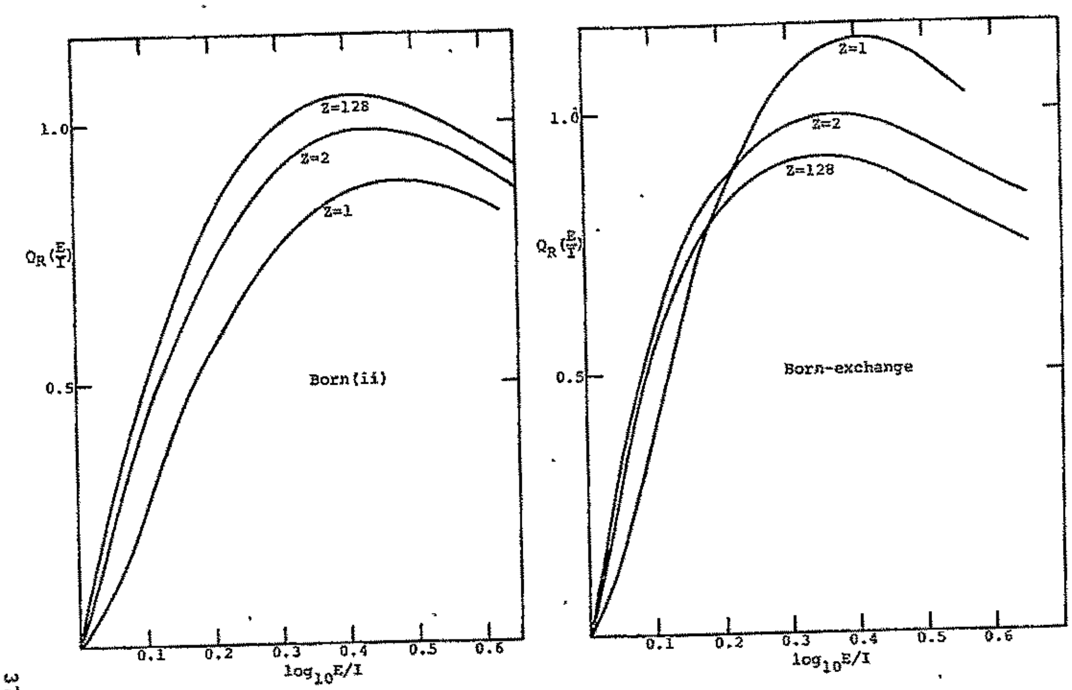

Figure (iv). Reduced ionization cross section for ionization from the 2s state for various Z values

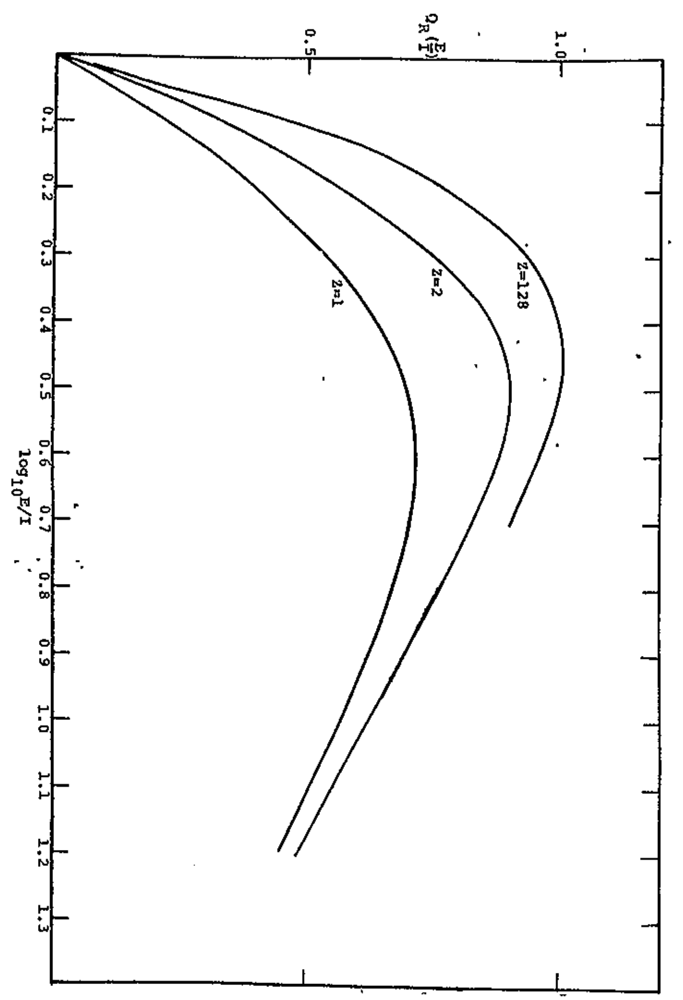

Figure (v). Reduced ionization cross section for ionization from the 1s state for various Z values

5. CONCLUSIONS

We have considered a number of approximations in the theory of ionizing collisions and applied these to the calculation of ionization cross sections for hydrogenic systems. Besides the interest in hydrogenic systems themselves, we have done so with a view to establishing which approximation might be best suited to the more difficult case of the ionization of complex atoms or ions by electron impact.

In comparing results for ionization from the ground state, it is seen that the Born-exchange results give the most satisfactory agreement with the experimental data. The agreement is particularly striking for the case of He^+ but less good for the case of hydrogen.

For hydrogen the effect of not treating the final state correctly as regards the Coulomb potentials might be thought to be a more severe limitation than for the case of a positive ion. Examination of the results in table VI, however, shows that the approximation adopted for the final state, although correct in its asymptotic behavior, does not lead to a cross section giving better agreement with experiment. It is notable that the exchange contribution in this approximation appears to be greatly overestimated, this being due to the fact that $z'(\underline{k},\underline{\chi})>z'(\underline{\chi},\underline{k})$. If one compares Q_d with the Born (ii) approximation, then it is seen that Q_d is indeed an improvement over the Born (ii) approximation. The situation would therefore seem to be that taking proper account of the Coulomb forces improves the calculation of $f(\underline{\chi},\underline{k})$

where $k>\chi$. In this region it is a good approximation to adopt the asymptotic (angle-dependent) Coulomb potential. Where $k<\chi$, however, this is no longer the case. Thus while $f(\underline{\chi},\underline{k})$ may be well determined for $k>\chi$, it is not a good approximation to write $g(\underline{\chi},\underline{k}) = f(\underline{k},\underline{\chi})$, since the success of this procedure relies on knowing $f(\underline{\chi},\underline{k})$ well for all $\underline{\chi}$ and $\underline{k}$. In the near-threshold region, however, the results using the angle-dependent potential are in accord with the theoretical threshold law derived by Rudge and Seaton (1965), while the Born (ii) and Born-exchange results are not. It should be mentioned, however, that there is an unresolved conflict between this theory and the experimental results of McGowan and Fineman (1965).

In the Born-exchange approximation the relative phase of the direct and exchange scattering amplitudes could be chosen at will. While theoretically inferior, therefore, it nevertheless yields more useful information about the cross section in those circumstances where the phase choice leads to compensation of errors. Just what those circumstances are is not clear. When one considers the results for ionization for the 2s state, it is seen that over the entire range in the case of hydrogen and over a part of the range for positive ions the effect of exchange increases the cross section. Also it appears that at high energies, as a result of exchange, the more highly ionized ions have a smaller cross section for ionization than the less highly ionized ions, in contrast to the situation for the ground state. This could be due to a weakness of the Born-exchange approximation, but there is no experimental information from which a conclusion can be drawn.

The situation therefore is not ideal, but we would nevertheless conclude that for highly ionized systems no substantial error should accrue for the case of the Born-exchange approximation, while the theoretically more sophisticated approximation which we have examined does not justify its added labor in terms of enhanced accuracy.

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13. ABSTRACT

Calculations of the ionization cross sections of hydrogen and of hydrogenic positive ions are described in which the initial state is either the ground or the excited 2s state. The first procedures used are the Born (II) and Born-exchange approximations. These results are compared with other theoretical calculations and with experimental data. It is seen that for the case of ionization of hydrogen from its ground state, none of the theoretical results is in good agreement with the experimental data. A certain defect of the theory is then corrected by adopting a third procedure for this case, in which an angle-dependent Coulomb potential is used in the description of the final state of the e-H ionization problem. It is then found that, despite the sounder theoretical footing of this latter calculation, no improved agreement with experimental data is obtained except in the near threshold region.

Convenient formulae are presented which represent the best data for the ionization cross sections and the associated reaction rates for the case of an initial Maxwellian distribution of velocities.

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